

Lipid membranes with an edge

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Consider a lipid membrane with a free exposed edge. The energy describing this membrane is quadratic in the extrinsic curvature of its geometry; that describing the edge is proportional to its length. In this note we determine the boundary conditions satisfied by the equilibria of the membrane on this edge, exploiting variational principles. The derivation is free of any assumptions on the symmetry of the membrane geometry. With respect to earlier work for axially symmetric configurations, we discover the existence of an additional boundary condition which is identically satisfied in that limit. By considering the balance of the forces operating at the edge, we provide a physical interpretation for the boundary conditions. We end with a discussion of the effect of the addition of a Gaussian rigidity term for the membrane.

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I. INTRODUCTION

A closed lipid membrane is described remarkably well by a geometrical hamiltonian. This hamiltonian is constructed as a sum of the scalars, truncated at an appropriate order, which characterize those features of the membrane geometry which are relevant. A term quadratic in the extrinsic curvature provides a measure of the energy penalty associated with bending [1, 2, 3, 4, 5]; any intrinsic tendency to bend one way and not the other is captured by a term linear in the extrinsic curvature [6].

The shape equation determining the equilibria of this membrane is a fourth-order non-linear elliptic PDE of the form $\nabla^2 K + 'K^3' = 0$, where ∇^2 is the Laplacian on the membrane, K is the sum of the principal curvatures, and by $'K^3'$ we mean a cubic polynomial in these curvatures [7]. Here, we would like to examine the boundary conditions which must supplement this equation when the membrane possesses a free edge. The energy cost associated with this edge is, to a good approximation, proportional to the exposed length. During the formation process, material will either be added to the edge or the edge will heal itself so as to form closed structures. However, unlike a simple soap film with a free edge, a lipid membrane does possess stable (cup shaped) equilibria [8]. An examination of such structures is a small but important step towards a fuller understanding of self assembly.

Our primary focus will be on the boundary geometry. We have a surface with a boundary and a certain energy penalty associated with it, a well defined problem in classical field theory. The boundary conditions are identified

by demanding that the energy be stationary for arbitrary deformations of the edge geometry. In distinction to earlier analytic treatments of this problem, we will relax the assumption that the membrane geometry be axially symmetric [8]. This is important not only for conceptual reasons. Generally, there will be no privileged parametrization such as that tailored to axial symmetry; in an axially symmetric geometry the edge itself is simply a circle. We find that there are three boundary conditions. As we will demonstrate one of these conditions, involving three derivatives of the embedding function, is satisfied identically in the axially symmetric limit. Therefore this limit cannot be considered as a reliable guide to the general case.

While the variational approach does capture the geometrical nature of the boundary conditions, the physical interpretation of these conditions still needs to be clarified. Ideally, one would like to interpret them in terms of the balance of forces operating at the edge. To do this in a way which does justice to the geometry, we identify the conserved Noether currents associated with the intrinsic translational invariance of the configuration [9]. The three, apparently unrelated, boundary conditions are now cast in terms of the three components of a single vector identity on the edge.

We finish with a discussion of the effect of a Gaussian rigidity term on a lipid membrane with edges. Whereas such a topological term does not alter the bulk shape equation, we show that it does modify the boundary conditions which apply to it in a way which will have consequences in the bulk. This extension is relevant in topology changing processes.

The outline of the paper is as follows. In Sect. II we consider the simple example of a surface tension dominated membrane. This allows us to establish our notation and to derive the boundary conditions in a simple context. In Sect. III, we derive the boundary conditions at the edge for a lipid membrane. We then specialize to

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axially symmetric configurations to compare our results in this limit with previous work on the subject. In Sect. IV, we consider the balance of the forces operating at the edge and we show how they are related to the boundary conditions. The effect of a Gaussian rigidity term to the membrane energy is the subject of Sect. V, where we obtain the appropriate modifications in the boundary conditions. We end with some remarks in Sect. VI.

II. SURFACE TENSION PITTED AGAINST EDGE TENSION

It is useful to examine first the simpler situation in which the membrane physics is dominated by surface tension, such as a soap film with a free edge. Let the membrane surface Σ have an area A , with boundary \mathcal{C} of length L , and the tension in the membrane bulk be a constant μ , and that on the edge σ . The energy is then given as a sum of two terms

$$F = \mu A + \sigma L. \quad (1)$$

Surface tension tends to decrease the membrane area; line tension to decrease the length of the free boundary. Without some further refinement this model does not admit stable equilibria. Suppose a hole is punctured in the film, then depending on its radius, either the hole will close healing the film, or grow and destroy it. An unstable equilibrium clearly exist when the radius is tuned to coincide with a critical value r_c . On dimensional ground, one would expect $r_c \approx \mu/\sigma$. (We will ignore stability here as our interest in this model is only as a point of reference for a lipid membrane.)

The membrane surface Σ is described by the embedding \mathbf{X} in three dimensional space R^3 as $\mathbf{x} = \mathbf{X}(\xi^a)$, where \mathbf{x} are coordinates for R^3 , and ξ^a coordinates for the surface ($a, b, \dots = 1, 2$). Its edge \mathcal{C} is embedded in turn as a curve on Σ as $\xi^a = Y^a(s)$ which we parametrize by its arclength s . We can now cast F as

$$F = \mu \int_{\Sigma} d^2\xi \sqrt{\gamma} + \sigma \oint_{\mathcal{C}} ds. \quad (2)$$

Here, the metric induced on Σ is given by $\gamma_{ab} = \mathbf{e}_a \cdot \mathbf{e}_b$, where $\mathbf{e}_a := \partial_a \mathbf{X}$ are tangent to the surface, $\gamma = \det \gamma_{ab}$, and $dA = \sqrt{\gamma} d^2\xi$. Note that we can also consider the direct embedding of the edge \mathcal{C} in R^3 , via $\mathbf{x} = \mathbf{Y}(s)$, where $\mathbf{Y} = \mathbf{X}(Y^a(s))$. The tangent to \mathcal{C} in R^3 is equivalently expressed in either of two ways: $\mathbf{t} = \mathbf{e}_a t^a$, where $t^a = \dot{Y}^a$; or $\mathbf{t} = \dot{\mathbf{Y}}$, where a dot denotes a derivative with respect to arclength s .

The energy is a functional of the embedding \mathbf{X} of Σ in R^3 . There is no need to vary the edge embedding Y^a independently: the Y^a are fixed by the constraint that the two embeddings agree, $\mathbf{Y} = \mathbf{X}$, on \mathcal{C} .

Equilibrium configurations are those at which the energy Eq.(1) is stationary. To derive the equations describing the equilibrium configurations of a membrane

described by this model, we first consider a variation of the embedding \mathbf{X} of the membrane $\mathbf{X} \rightarrow \mathbf{X} + \delta\mathbf{X}$. We let \mathbf{n} denote the unit normal to the surface Σ . We decompose the displacement with respect to the spatial basis adapted to Σ , $\{\mathbf{e}_a, \mathbf{n}\}$, as,

$$\delta\mathbf{X} = \Phi^a \mathbf{e}_a + \Phi \mathbf{n}. \quad (3)$$

We now have that the induced metric varies according to (see *e.g.* [9])

$$\delta_X \gamma_{ab} = 2K_{ab}\Phi + \nabla_a \Phi_b + \nabla_b \Phi_a, \quad (4)$$

where K_{ab} denotes the extrinsic curvature tensor,

$$K_{ab} = \mathbf{e}_b \cdot \partial_a \mathbf{n}, \quad (5)$$

and ∇_a is the covariant derivative on Σ compatible with γ_{ab} . The derivative terms in the variation of γ_{ab} are its Lie derivative along the tangential vector field, Φ^a . The variation of A is

$$\begin{aligned} \delta_X A &= \int_{\Sigma} dA [K \Phi + \nabla_a \Phi^a] \\ &= \int_{\Sigma} dA K \Phi + \oint_{\mathcal{C}} ds l^a \Phi_a. \end{aligned} \quad (6)$$

The mean extrinsic curvature, $K = K_{ab}\gamma^{ab}$. The second line follows from the preceding one using Stoke's theorem. Here l^a is the outward pointing normal to \mathcal{C} on Σ . Only the normal projection Φ of the variation plays a role in determining the bulk equilibrium of the membrane. This is true generally, regardless of the model. In this particular model, however, there is no boundary term associated with the bulk normal displacement Φ . As we will see, this is not generally true — a happy accident when the energy is truncated at the area term. On the other hand, the tangential bulk variation Φ^a always gives only a boundary term. This is a consequence of the fact that a tangential deformation corresponds in the bulk to an infinitesimal reparametrization of the surface. There is however a physical displacement of the boundary. In fact, the boundary contribution to Eq.(6) is easily identified as the change in the surface area of Σ under a normal deformation of its boundary, $\delta Y^a = (l^b \Phi_b) l^a$, which at each point is directed along the tangent plane of Σ at that point. The projection of Φ^b onto the edge \mathcal{C} itself, $t^a \Phi_a$, does not contribute.

Let us turn now to the variation of the edge embedding \mathbf{Y} induced by the bulk variation $\delta\mathbf{X}$. It can be decomposed with respect to a basis adapted to both embeddings, \mathbf{X} and \mathbf{Y} , given by $\{\mathbf{t}, \mathbf{l}, \mathbf{n}\}$, where $\mathbf{l} = \mathbf{e}_a l^a$. Thus at the edge we set

$$\delta\mathbf{Y} = \phi \mathbf{t} + \psi \mathbf{l} + \Phi \mathbf{n}, \quad (7)$$

where the edge and bulk components are identified by continuity, $\psi = l^a \Phi_a$ and $\phi = t^a \Phi_a$. Modulo a divergence associated with a reparametrization of the boundary which involves the tangential component ϕ that we

can safely discard, we have for the variation of the infinitesimal arclength

$$\delta_Y ds = ds (\kappa \psi + K_{\parallel} \Phi), \quad (8)$$

where we have used the fact that

$$\dot{\mathbf{t}} = -\kappa \mathbf{l} - K_{\parallel} \mathbf{n}. \quad (9)$$

Here κ is the geodesic curvature of \mathcal{C} associated with its embedding in Σ , and we have defined $K_{\parallel} = K_{ab} t^a t^b$. The unconventional minus sign in the first term of Eq. (9) comes about because \mathbf{l} is the *outward* normal to \mathcal{C} on Σ , *i.e.* $\dot{t}^a = -\kappa l^a$.

The corresponding deformation in L is then given by

$$\delta_Y L = \oint_{\mathcal{C}} ds (\kappa \psi + K_{\parallel} \Phi). \quad (10)$$

Summing the two contributions (6) and (10) to the variation of the energy F , as given by (1), we find

$$\delta_X F = \mu \int_{\Sigma} dA K \Phi + \oint_{\mathcal{C}} ds [(\mu + \sigma \kappa) \psi + \sigma K_{\parallel} \Phi]. \quad (11)$$

The bulk equilibrium is a minimal surface unaffected by the boundary, satisfying $K = 0$. On the boundary, the projections along the normals to the edge, ψ and Φ , represent independent deformations, so that stationarity of F requires the vanishing of the corresponding coefficients. We thus read off the two boundary conditions:

$$\sigma \kappa + \mu = 0, \quad (12)$$

$$\sigma K_{\parallel} = 0. \quad (13)$$

The first tells us that the geodesic curvature of the edge as embedded in the membrane is constant. The second simply enforces the vanishing of K_{\parallel} at the edge. Note that the completeness of the basis $\{\mathbf{t}, \mathbf{l}\}$ of tangent vectors on Σ at \mathcal{C} , $\gamma^{ab} = t^a t^b + l^a l^b$, permits us to express the mean curvature at the edge as $K = K_{\parallel} + K_{\perp}$, where $K_{\perp} = K_{ab} l^a l^b$. Thus modulo the bulk equilibrium $K = 0$, the boundary condition (13) can be alternatively expressed as $K_{\perp} = 0$. The only potentially non vanishing component of K_{ab} on the edge is the off-diagonal component, $K_{\parallel\perp} = t^a l^b K_{ab}$.

For this particular model our approach has been heavy-handed; the boundary conditions we have written down are an elaborate way to express the simple vector identity

$$\sigma \dot{\mathbf{t}} = \mu \mathbf{l}, \quad (14)$$

which equates the change in the tension over the interval Δs along the edge, $\sigma \Delta \mathbf{t}$, to the force due to surface tension acting on the edge, $\mu \mathbf{l} \Delta s$. The apparent mismatch in counting (three versus two) is accounted for by noting that the projection of Eq.(14) along \mathbf{t} is an identity. For higher order models, as we will see, this projection will not be vacuous.

Note that had we N sheets conjoined on a single edge, Eq.(14) gets modified in an obvious way:

$$\sigma \dot{\mathbf{t}} = \mu \sum_{i=1}^N \mathbf{l}_i, \quad (15)$$

where \mathbf{l}_i is the vector normal to the edge which is tangent to the i^{th} sheet. Eq.(15) provides a generalization of the Neumann rule for soap bubble clusters at a Plateau border [10] to accomodate line tension on the edge. A simple application is considered in [11].

III. LIPID MEMBRANE WITH AN EDGE

A lipid membrane is modeled by a phenomenological energy quadratic in the extrinsic curvature of the surface. Let us write this as

$$F_b = \int_{\Sigma} dA \mathcal{F}(\gamma^{ab}, K_{ab}), \quad (16)$$

i.e. \mathcal{F} depends at most on the extrinsic curvature, and not, for example, on its derivative $\nabla_a K_{bc}$. In particular, we will focus on the model described by the Helfrich energy density

$$\mathcal{F} = \alpha(K - K_0)^2 + \mu. \quad (17)$$

The spontaneous curvature K_0 is a constant, as is the bending rigidity α . The constant μ is interpreted here as the Lagrange multiplier implementing the constraint on the membrane area. We will discuss the addition of a Gaussian rigidity term in the next section.

The energy of the bulk and the edge is

$$F = F_b + \sigma L. \quad (18)$$

The shape equation describing the equilibrium in the bulk, which is derived from the extremization of the energy (17)

$$\alpha[-2\nabla^2 K + 2(K - K_0)\mathcal{R} + (K_0^2 - K^2)K] + \mu K = 0, \quad (19)$$

is well known [7]. The structure of this equation has been discussed in detail elsewhere [9], where a novel derivation is also provided. The scalar curvature \mathcal{R} appearing in Eq.(19) is related to the extrinsic curvature through the Gauss-Codazzi equation,

$$\mathcal{R} = K^2 - K_{ab} K^{ab}. \quad (20)$$

Under a tangential deformation of the surface, $\delta_{\parallel} \mathbf{X} = \Phi^a \mathbf{e}_a$, the energy density transforms as a divergence which is transferred to the boundary,

$$\delta_{\parallel} F_b = \oint_{\mathcal{C}} ds \mathcal{F} l_a \Phi^a. \quad (21)$$

This is because the local scalar energy density \mathcal{F} transforms as

$$\delta_{\parallel} \mathcal{F} = \Phi^a \partial_a \mathcal{F}. \quad (22)$$

The details of \mathcal{F} do not enter. Note that Eq.(21) agrees with the corresponding expression for the area with $\mathcal{F} = 1$. As before, this boundary term induces a source into the boundary Euler-Lagrange equation. For an edge with a line tension σ , we get the first boundary condition, due to a deformation along the normal \mathbf{l} , ψ ,

$$\sigma\kappa + \mathcal{F} = 0, \quad (23)$$

where we have used Eqs. (10) and (21). This should be compared with Eq.(12) to which it reduces if $\mathcal{F} = \mu$, a constant. This boundary condition relates the geometry of the edge to the extrinsic curvature of the membrane evaluated at the boundary.

We now examine a normal deformation of the surface Σ , $\delta_\perp \mathbf{X} = \Phi \mathbf{n}$. The shape equation (19) determining the local membrane equilibrium is obtained by demanding that the energy be stationary with respect to normal deformations of Σ which may or may not vanish on the boundary. As such this equation cannot be affected by the addition of a boundary. To determine the boundary conditions we need to extend the support of the variation to include the boundary. We have that the normal variation of the bulk energy can be written as

$$\delta_\perp F_b = \int dA [\mathcal{F}K\Phi + 2\Gamma_{ab}K^{ab}\Phi + \mathcal{F}^{ab}\delta_\perp K_{ab}], \quad (24)$$

where $\Gamma_{ab} = \partial\mathcal{F}/\partial\gamma^{ab}$ and $\mathcal{F}^{ab} = \partial\mathcal{F}/\partial K_{ab}$. The boundary term we wish to identify in $\delta_\perp F_b$ originates in the $\delta_\perp K_{ab}$ term in this expression. We recall that the extrinsic curvature transforms as follows under a normal deformation of Σ (see *e.g.* [9]):

$$\delta_\perp K_{ab} = -\nabla_a \nabla_b \Phi + K_{ac}K^c{}_b \Phi. \quad (25)$$

We thus have that

$$\delta_\perp F_b = \int dA [\mathcal{E}\Phi + \nabla_a (\Phi \nabla_b \mathcal{F}^{ab} - \mathcal{F}^{ab} \nabla_b \Phi)], \quad (26)$$

where we have defined the Euler-Lagrange derivative

$$\mathcal{E} = (-\nabla_a \nabla_b + K_{ac}K^c{}_b)\mathcal{F}^{ab} + \mathcal{F}K + 2\Gamma_{ab}K^{ab}. \quad (27)$$

Thus, modulo the bulk shape equation, $\mathcal{E} = 0$, we get that the boundary contribution is

$$\delta_\perp F_b = \oint_{\mathcal{C}} ds l_a [\Phi \nabla_b \mathcal{F}^{ab} - \mathcal{F}^{ab} \nabla_b \Phi]. \quad (28)$$

The terms proportional to $\nabla_a \Phi$ and Φ are not independent: the projection of $\nabla_a \Phi$ along the edge is completely determined once Φ is specified on \mathcal{C} . To decompose $\delta_\perp F$ into two independent parts we proceed as follows: we first decompose $\nabla_a \Phi$ into its normal and tangential parts with respect to \mathcal{C} ,

$$\nabla_a \Phi = l_a \nabla_\perp \Phi + t_a \dot{\Phi}, \quad (29)$$

where we have defined $\nabla_\perp = l^a \nabla_a$. We now perform an integration by parts on the $\dot{\Phi}$ term to obtain for the second term on the right hand side of Eq.(28)

$$\oint_{\mathcal{C}} ds l_a \mathcal{F}^{ab} \nabla_b \Phi = \oint_{\mathcal{C}} ds \left[l_a l_b \mathcal{F}^{ab} \nabla_\perp \Phi - \Phi \frac{d}{ds} (l_a \mathcal{F}^{ab} t_b) \right], \quad (30)$$

where we have discarded a total derivative term with respect to arclength. In this way we succeed in isolating the independent normal variations at the boundary, the coefficients of Φ and $\nabla_\perp \Phi$.

From Eqs. (10), (28), (30), we obtain that the total boundary contribution of the normal variations is

$$\delta_\perp F_b = \oint_{\mathcal{C}} ds \left\{ -l_a l_b \mathcal{F}^{ab} \nabla_\perp \Phi + \left[l_a \nabla_b \mathcal{F}^{ab} + \frac{d}{ds} (l_a \mathcal{F}^{ab} t_b) + \sigma K_\parallel \right] \Phi \right\}, \quad (31)$$

so that we can immediately read off the two boundary conditions which supplement Eq. (23),

$$l_a \nabla_b \mathcal{F}^{ab} + \frac{d}{ds} (l_a \mathcal{F}^{ab} t_b) + \sigma K_\parallel = 0, \quad (32)$$

$$l_a l_b \mathcal{F}^{ab} = 0. \quad (33)$$

The first is of third order in derivatives of the embedding functions. This is consistent with the fact that the shape equation (19) is of fourth order. Using the decomposition of the covariant derivative (29), it can be written in the alternative form

$$l_a l_b \nabla_\perp \mathcal{F}^{ab} + 2 \frac{d}{ds} (l_a \mathcal{F}^{ab} t_b) + \kappa (l_a l_b - t_a t_b) \mathcal{F}^{ab} + \sigma K_\parallel = 0. \quad (34)$$

In the case of a membrane described by the Helfrich Hamiltonian (17) with an edge the third boundary condition (33) implies

$$K = K_0, \quad (35)$$

on the edge — the rigid membrane necessarily has a constant mean curvature at the edge equal to its spontaneous value. This is entirely independent of the tensions, μ or σ , or of the rigidity modulus. If $K_0 = 0$, the membrane is minimal at its edge.

The second boundary condition (32) is of Robin type. For any \mathcal{F} which is a function only of K , we have that $\mathcal{F}^{ab} \propto \gamma^{ab}$, so that the middle term in (32) vanishes,

$$l_a \mathcal{F}^{ab} t_b = 0, \quad (36)$$

and the boundary condition reduces to

$$2\alpha \nabla_\perp K + \sigma K_\parallel = 0. \quad (37)$$

This equation determines the normal derivative of K in terms of the component of the extrinsic curvature tangent to the edge. It does not involve the surface tension

μ . We emphasize that its existence seems to have gone unnoticed.

The first boundary condition, Eq.(23), together with Eq.(35), implies that on the edge

$$\sigma\kappa + \mu = 0. \quad (38)$$

The geodesic curvature of a loaded boundary is completely fixed by the ratio of the tensions in exactly the same way as in the previous section for soap bubbles, see Eq. (12). If $\mu = 0$ the edge is necessarily a geodesic of the bulk geometry.

If the line tension on the boundary vanishes, $\sigma = 0$, the consistency of Eq.(35) with (23) requires that $\mu = 0$ also. Furthermore Eq.(37) implies $\nabla_\perp K = 0$ on the boundary. But the unique solution satisfying the two boundary conditions $K = K_0$ and $\nabla_\perp K = 0$ is $K = K_0$ everywhere. One way to see this is to construct the Gaussian normal coordinates adapted to the edge, (l, s) , where l is the length of the geodesic which intersects the edge normally. With respect to this system of coordinates, the Laplacian assumes the form $\nabla^2 = \partial_l^2 + \kappa\partial_l + \partial_s^2$ in the neighborhood of the edge. Thus, modulo the boundary conditions, $\nabla^2 K = \partial_l^2 K$ on the edge. But Eq.(19) implies that $\nabla^2 K = 0$ there so that $\partial_l^2 K$ and all higher derivatives vanish. If K is analytic in l , then $K = K_0$. If $\mu \neq 0$, there is no such constraint. The geometry is very severely constrained by the boundary conditions.

Let us now examine an axially symmetric membrane with an axially symmetric edge. With respect to cylindrical polar coordinates $\{\rho, z, \varphi\}$ on R^3 , the membrane is described by $\rho = R(\ell)$, $z = \mathcal{Z}(\ell)$ where $\mathcal{Z}'^2 + R'^2 = 1$.

ℓ is the arc length along a curve with fixed φ , and the primes denote a derivative with respect to ℓ . The intrinsic geometry of Σ is described by the line element

$$d\tau^2 = d\ell^2 + R^2(\ell)d\varphi^2, \quad (39)$$

We can write the extrinsic curvature in a form consistent with axial symmetry as

$$K_{ab} = \ell_a \ell_b K_\ell + (\gamma_{ab} - \ell_a \ell_b) K_R, \quad (40)$$

where K_ℓ and K_R are two spatial scalars which we identify as the principal curvatures of the embedding of Σ in R^3 , ℓ^a is the outward pointing unit normal to the circle of fixed ℓ , $\ell^a = (1, 0)$. The mean curvature is $K = K_\ell + K_R$. To evaluate the principal curvatures, it is convenient to define Θ as the angle which the tangent to a curve of fixed φ makes with the cylindrical radial direction:

$$\frac{d\mathcal{Z}}{dR} = \tan \Theta. \quad (41)$$

We then have $\mathcal{Z}' = \sin \Theta$, and $R' = \cos \Theta$, so that the principal curvatures are

$$K_\ell = \Theta', \quad K_R = \frac{\sin \Theta}{R}. \quad (42)$$

Axial symmetry implies that the fourth order shape equation can be integrated to provide a third order equation for R as a function of ℓ . It has been shown elsewhere ([12, 13], see also [9]) that this equation takes the form

$$-2\alpha \cos \Theta \left(\Theta' + \frac{\sin \Theta}{R} \right)' + \alpha \left(\Theta' + \frac{\sin \Theta}{R} \right) (\Theta' - \frac{\sin \Theta}{R}) \sin \Theta + 2\alpha K_0 \frac{\sin^2 \Theta}{R} - (\mu + \alpha K_0^2) \sin \Theta = 0. \quad (43)$$

If the boundary \mathcal{C} is also axially symmetric so that it coincides with a fixed value of ℓ then $\ell^a = \ell^a$, $K_\parallel = K_R$, $K_\perp = K_\ell$ and $K_{\parallel\perp} = 0$. It is simple to show that $\kappa = -R'/R$. We thus have for the boundary conditions, Eqs.(35) and (38),

$$\Theta' + \sin \Theta / R = K_0, \quad \sigma R' = \mu R. \quad (44)$$

The remaining boundary condition, Eq.(37), of third order in derivatives appears to present a problem: a third order ODE does not admit third order boundary conditions. The inconsistency, however, is only apparent: on the boundary, the shape equation Eq.(43) itself reproduces, modulo Eqs.(44), the troublesome boundary condition Eq.(37). Our analysis is thus completely consistent with the axially symmetric analysis of [8] where the boundary conditions Eqs.(23) and (33) are derived. It is worth stressing, however, that potential pitfalls of using the axially symmetric problem as a guide to the more

general problem. The boundary condition (32) is a non-trivial constraint on the geometry which is not already encoded in the shape equation for non-axially symmetric configurations.

IV. BALANCE OF FORCES

In this section, we consider the balance of the forces operating at the edge. This provides the missing intuition on the physical origin of the boundary conditions we have derived in the previous section.

Consider a point on the edge. In equilibrium, the tension \mathbf{g} must satisfy

$$\dot{\mathbf{g}} = \mathbf{f}^a l_a. \quad (45)$$

Here \mathbf{f}^a is the membrane stress tensor so that $\mathbf{f}^a l_a$ is the ‘surface tension’ acting on the edge due to unbalanced

stresses in the bulk at its boundary. In [9], it was shown that the bulk stress tensor for the model defined by the Helfrich energy (17) can be expressed in the form

$$\mathbf{f}^a = [2\alpha K(K^{ab} - \frac{K}{2}\gamma^{ab}) - 2\alpha K_0(K^{ab} - K\gamma^{ab}) - (\mu + \alpha K_0^2)\gamma^{ab}]\mathbf{e}_b - 2\alpha\nabla^a K\mathbf{n}. \quad (46)$$

Thus its projection along the normal to the edge l^a is

$$\mathbf{f}^a l_a = \{2\alpha(K - K_0)K_\perp - \alpha(K - K_0)^2 - \mu\}\mathbf{l} + 2\alpha(K - K_0)K_{\parallel\perp}\mathbf{t} - 2\alpha\nabla_\perp K\mathbf{n}. \quad (47)$$

In addition, as we have seen in Sect. II,

$$\mathbf{g} = -\sigma\mathbf{t}. \quad (48)$$

Using Eq. (9) for $\dot{\mathbf{t}}$, we read off the three components of Eq.(45),

$$\sigma\kappa = 2\alpha(K - K_0)K_\perp - \alpha(K - K_0)^2 - \mu, \quad (49)$$

$$\sigma K_\parallel = -2\alpha\nabla_\perp K, \quad (50)$$

$$0 = 2\alpha(K - K_0)K_{\parallel\perp}, \quad (51)$$

respectively along \mathbf{l} , \mathbf{n} , and \mathbf{t} . The condition (50) coincides with the boundary condition (37). If $K_{\parallel\perp} \neq 0$, Eq.(51) implies that $K = K_0$. The remaining boundary condition (49) then coincides with a linear combination of the boundary conditions (35) and (38). In the axially symmetric geometry, however, $K_{\parallel\perp}$ does vanish so that (51) does not imply $K = K_0$ as it stands. One needs then to appeal to the integrated shape equation (43), which together with (49) and (50) reproduce $K = K_0$.

We thus have identified a very simple (if heavily disguised) physical interpretation of the boundary conditions. In particular, in this approach, the boundary condition $K = K_0$ emerges as the vanishing of the stress induced by the bulk along the edge. Note that the variational approach did not rely on the identification of projections. Indeed, the boundary condition corresponding to the projection along \mathbf{t} was originally identified by demanding stationary energy for independent boundary variations of $\nabla_\perp\Phi$.

We also note that the form of Eq.(45) implies the integrability condition,

$$\oint_C ds \mathbf{f}^a l_a = 0 \quad (52)$$

on the edge. The existence of these three extremely non-trivial conditions is far from obvious in our previous approach.

One can say more. Take the equation, $\nabla_a \mathbf{f}^a = 0$, describing the conservation of the stress tensor. dot it into \mathbf{X} and integrate over the membrane surface. We get

$$\int dA \nabla_a (\mathbf{X} \cdot \mathbf{f}^a) = \int dA \mathbf{e}_a \cdot \mathbf{f}^a. \quad (53)$$

Working on the right, we have

$$\begin{aligned} \int dA \nabla_a (\mathbf{X} \cdot \mathbf{f}^a) &= \oint ds \mathbf{X} \cdot l_a \mathbf{f}^a \\ &= \oint ds \mathbf{X} \cdot \dot{\mathbf{g}} \\ &= - \oint ds \mathbf{t} \cdot \mathbf{g} \\ &= \sigma L, \end{aligned} \quad (54)$$

where we have used Eq.(45) on the second line, as well as Eq.(48) on the last line. On the other hand, if we write $\mathbf{f}^a = f^{ab}\mathbf{e}_b + f^a\mathbf{n}$, then

$$\int dA \mathbf{e}_a \cdot \mathbf{f}^a = \int dA f^a_a. \quad (55)$$

We note that the bending energy $\int dA K^2$ is a conformal invariant, and so does not contribute to the trace f^a_a . We have $f^a_a = 2(\alpha K_0(K - K_0) - \mu)$, so that

$$2\mu A - 2\alpha K_0 \int dA (K - K_0) + \sigma L = 0. \quad (56)$$

This condition is useful for identifying the sign associated with the multipliers. For example, if $K_0 = 0$, it is clear that μ is necessarily negative.

V. GAUSSIAN RIGIDITY

The geometrical scalars we can construct with dimension $[\text{Length}]^{-2}$ are \mathcal{R} , K^2 and $K_{ab}K^{ab}$. The Gauss-Codazzi equation (20) tells us that the three scalar invariants \mathcal{R} , K^2 and $K_{ab}K^{ab}$ are not independent. In addition, the Gauss-Bonnet functional

$$I = \int_\Sigma dA \mathcal{R} \quad (57)$$

is a topological invariant if the membrane is closed. More generally for an open membrane,

$$I = \int_\Sigma dA \mathcal{R} + 2 \oint_C ds \kappa \quad (58)$$

is a topological invariant. A consequence is that if a Gaussian rigidity term is included in the energy a line rigidity $\oint_C ds \kappa$ is necessarily induced along its boundary.

To obtain the variation of the Gaussian term, we need to know how the scalar curvature varies. Its tangential deformation is straightforward; to determine its normal deformation, we exploit Eq.(20) and with it the technology developed Sects. II and III.

Consider now a Gaussian rigidity addition to the bulk energy, so that

$$F = F_b + \beta \int dA \mathcal{R}, \quad (59)$$

Whereas the bulk shape equation is unmodified, all three boundary conditions are changed:

$$\alpha(K - K_0)^2 + \beta\mathcal{R} + \mu + \sigma\kappa = 0, \quad (60)$$

$$2\alpha\nabla_\perp K - 2\beta\dot{K}_{\parallel\perp} + \sigma K_{\parallel} = 0, \quad (61)$$

$$\alpha(K - K_0) + \beta K_{\parallel} = 0. \quad (62)$$

We note that the Gauss-Codazzi equation (20) allows us to express \mathcal{R} in terms of the projections of K_{ab} with respect to the edge, $\mathcal{R} = 2(K_{\parallel}K_{\perp} - K_{\parallel\perp}^2)$. Eq.(60) is quadratic in the extrinsic curvature. Eqs.(61) and (62) by contrast are linear relationship between K_{\perp} and K_{\parallel} .

Note that, unlike the case of the pure Helfrich model, the central term in Eq.(61) does not vanish in general. However, it does vanish in an axially symmetric geometry (with axially symmetric edge), $K_{\parallel\perp} = 0$. More generally, we have the integral statement

$$\oint_C ds [2\alpha\nabla_\perp K + \sigma K_{\parallel}] = 0. \quad (63)$$

In an axially symmetric geometry one can check that, modulo the lower order boundary conditions (60) and (62), Eq.(43) reproduces Eq.(61) on the boundary.

Let us consider now the balance of the forces in this case. The Gaussian term makes no contribution to \mathbf{f}^a [9]. Naively reinvoking Eq.(45) would appear to suggest that this term cannot modify the boundary conditions, in contradiction with what we have just derived. However, with a general function \mathcal{F} and in particular for $\beta\mathcal{R}$, the term $d/ds(l_a\mathcal{F}^{ab}t_b)\Phi$ appearing in its normal variation (see Eq.(30)) will be non-vanishing, and it is no longer appropriate to discard a total derivative as we did in deriving Eq. (30). For consistency, we claim therefore that we need to modify Eq.(45) as follows:

$$\mathbf{g} \rightarrow \mathbf{g} - l_a\mathcal{F}^{ab}t_b\mathbf{n}. \quad (64)$$

For Gauss-Bonnet, the second term reads $-2\beta K_{\parallel\perp}\mathbf{n}$. This mysterious term is precisely the tension associated with the edge energy $\oint_C ds \kappa$. The projections of Eq.(45) along \mathbf{l} , \mathbf{n} and \mathbf{t} respectively then read

$$\alpha [(K - K_0)^2 - 2(K - K_0)K_{\perp}] - 2\beta K_{\parallel\perp}^2$$

$$+ \sigma\kappa + \mu = 0, \quad (65)$$

$$2\alpha\nabla_\perp K - 2\beta\dot{K}_{\parallel\perp} + \sigma K_{\parallel} = 0, \quad (66)$$

$$2K_{\parallel\perp}[\alpha(K - K_0) + \beta K_{\parallel}] = 0, \quad (67)$$

where we have used the fact that, at the edge,

$$\dot{\mathbf{n}} = K_{\parallel}\mathbf{t} + K_{\perp}\mathbf{l}. \quad (68)$$

As was the case in the previous section, these coincide with the boundary conditions (60), (61), (62) when $K_{\parallel\perp} \neq 0$.

VI. CONCLUSIONS

Whereas for a soap film, it is very simple to identify the forces operating on the edge, and so read off the boundary conditions on the bulk geometry, such an approach is less obvious for a membrane. However, we have demonstrated how simple geometrical and variational arguments may be exploited to derive the boundary conditions on the lipid membrane geometry. We have made no restrictive assumptions about the symmetry of the configuration. We then showed how these boundary conditions emerge from a balance of forces projected along a basis of vectors adapted to the edge.

We plan at a future date to examine the axially symmetric shape equation subject to the Gauss-Bonnet modified boundary conditions. Matching observed configurations with solutions of the shape equation in this more general setting provides a method, at least in principle, for determining the values of the two bulk rigidity moduli.

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- [1] D. Nelson, T. Piran, and S. Weinberg, eds., *Statistical Mechanics of Membranes and Surfaces*, vol. 5 (World Scientific, Singapore, 1989), (Proceedings of the Jerusalem Winter School for Theoretical Physics).
 - [2] L. Peliti, in *Fluctuating Geometries in Statistical Physics and Field Theory (Les Houches 1994)*, edited by F. David, P. Ginsparg, and J. Zinn-Justin (Elsevier Science B.V., 1996).
 - [3] S. Safran, *Statistical Physics of Surfaces, Interfaces, and Membranes* (Reading UK, Addison Wesley, 1994).
 - [4] R. Lipowsky and E. Sackmann, *Structure and Dynamics of Membranes, Vol. 1 and 2* (Handbook of Biological Physics, Elsevier Science B.V., 1995).
 - [5] U. Seifert, *Adv. in Phys.* **46**, 13 (1997).
 - [6] W. Helfrich, *Z. Naturforsch.* **C28**, 693 (1973).
 - [7] O.-Y. Zhong-Can and W. Helfrich, *Phys. Rev. Lett.* **59**, 2486 (1987).
 - [8] D. Boal and M. Rao, *Phys. Rev. A* **46**, 3037 (1992).
 - [9] R. Capovilla and J. Guven, *Stresses in lipid membranes* cond-mat/0203148.
 - [10] D. Weaire and S. Hutzler, *The Physics of Foams* (Oxford Univ. Press, 1999).

- [11] R. Capovilla and J. Guven, *Limiting pressures in coalesced soap bubbles* (2002), (preprint).
- [12] W. Zheng and J. Liu, Phys. Rev. E **48**, 2856 (1993).
- [13] B. Božič, S. Svetina, and B. Žekš, Phys. Rev. E **55**, 5843 (1997).